CHAPTER V

INTRODUCTION TO MODELING ACTIVITIES

A. INTRODUCTION

Mathematical modeling of ecosystems is a relatively young technique which, in simplest terms, seeks to simulate actual environmental conditions in a numerically quantifiable fashion. Ideally, a model is a dynamic conceptual framework which enables a clearer understanding of major factors affecting existing states within an ecosystem. Under certain conditions, some numerical simulations offer the added advantage of using data on existing environmental states, coupled with ecosystem process information, to enable predictions of future trends and tendencies. Quite logically, the predictive capability of such a tool is only as good as the conceptual framework of the model, the data set upon which it is based, the assumptions required to develop the model, and the extent to which the model has been both calibrated and verified.

Two types of models were developed in the UGLCCS. The first type of model is based on mass balance calculations. The second type of model is a process-oriented model. Both types of modeling efforts are valuable for indicating needed research, remedial and regulatory actions.

With sufficient data, mass balance calculations are useful for determining (1) whether an area is a source or sink of contaminants, and (2) the relative importance of known and unknown contaminant sources. Mass balance calculations were made for a number of water quality parameters in Lake St. Clair and the Detroit River (including the Trenton Channel, Table V-1). The mass balances calculated for these systems represent order of magnitude "snapshots" of contaminant fluxes since measurements were made during short time intervals only. Annual mass balances cannot be inferred from these calculations unless specifically noted.

TABLE V-1

Mass balance calculations performed on the Upper Great Lakes Connecting Channels.

Location	Date(s)	Parameters
St. Clair R.	Aug., Sept., Oct., 1985	Organics (concentration profiles only)
Lake St. Clair	July 21-29, 1986	Metals, Organics, Total Phosphorus
Detroit River	April 21-29, 1986 (SMB I)	Metals, Organics, Nutrients, Chlorides, Suspended Solids
	July 25 - August 5, 1986 (SMB II)	Metals, Organics, Nutrients, Chlorides, Suspended Solids
Trenton Channel	May 6-7, 1986	Metals, Organics, Nutrients, Chlorides, Suspended Solids
	August 26-27, 1986	Metals, Organics, Nutrients, Chlorides, Suspended Solids

Process-oriented models are based on mechanistic relationships (e.g. contaminant-sediment interactions) and represent a working hypothesis of how a dynamic system works. Process-oriented models are useful for (1) understanding the relative importance of processes that affect contaminant fate, and (2) given proper calibration and verification, for answering "what if" questions (e.g., if a particular contaminant is added to a system, where will it go, how long will it stay, what physical-chemical form will it be in, and what organism exposure might occur?). Models describing a variety of physical, chemical and biological processes were developed for the St. Marys River, the St. Clair River, Lake St. Clair, the Detroit River and the Trenton Channel (Table V-2).

TABLE V-2

Process models developed for the Upper Great Lakes Connecting Channels Study.

Location	Type of Model
St. Marys River	- 3-D steady state finite element hydrodynamic (upper river) - Steady state, depth averaged, mixing model (lower river) - Contaminant fate model (driven by hydrodynamic models, above)
St. Clair River	- Unsteady flow model with flow separation around islands - Steady state depth averaged mixing model - Contaminant fate model (water column only) - Contaminant fate model (TOXIWASP-based water and sediments)
Lake St. Clair	- Water level models (hydrodynamic and empirical) - Currents (predicts mean and daily currents) - Particle transport model - 3-D finite element flow field model - Waves and sediment settling and resuspension - Contaminant fate, 2-D model (TOXIFATE) - Contaminant fate, 2-D model (TOXIWASP-based) - Contaminant fate, 1 box kinetic model
Detroit River	- 2-D plume model of water and contaminant discharge from Detroit's sewage treatment plant
Trenton Channel	- 3-D hydrodynamic and toxicity transport model

B. METHODS

1. Mass Balance Calculations

Mass is a conservative property. As such, a material balance framework can be applied to a control volume (i.e., water body) where, assuming conservative behaviour and steady state conditions, the change in mass of the system can be described as:

$$D = W_{out} - W_{in}$$

W_{in} is the sum of all loads (flux) coming into the control volume (mass/time). W_{out} is the mass flux leaving the control volume. If all loadings into the system are accounted for and the mass flux leaving the system is known, then "D" should equal zero for a conservative substance. In general, if D is not zero, then the control volume is either a sink ($D<0$) or a source ($D>0$) of the substance. For substances that "leave" the system through volatilization or degradation it is important to note that a $D<0$ does not necessarily mean that the substance is accumulating in the control volume. A process-oriented calculation would be needed to define how much substance was lost through volatilization or degradation before an accurate estimate of accumulation could be made. Figure V-1 provides examples of mass balance calculations and interpretations based on various situations.

In the Connecting Channels where horizontal flow (advection) dominates, the W terms can be computed from:

$$W = Q * C$$

Where, W is mass flux (M/T)
Q is the flow rate (L^3/T), and
C is the concentration (M/L^3).

There are two sources of error in calculating W. First, there are analytical errors associated with measurement of Q and C. Second, errors can be introduced by inadequate temporal and spatial sampling. Ideally, analytical errors would be non-existent and sampling of Q and C would be continuous at all locations. This is never the case, however, so W is always an estimate of the true load. Annual loads would ideally be calculated based on continuous measurements of Q and C throughout a year period. However, Q and C measurements might have been taken on a weekly basis only. Annual loads calculated with weekly information will be less certain than if the measurements were continuous.

Contaminant concentration data are sometimes reported as non-detectable or below the detection limit. This does not imply that the contaminant is not present in the sample, but merely that it cannot be quantified.

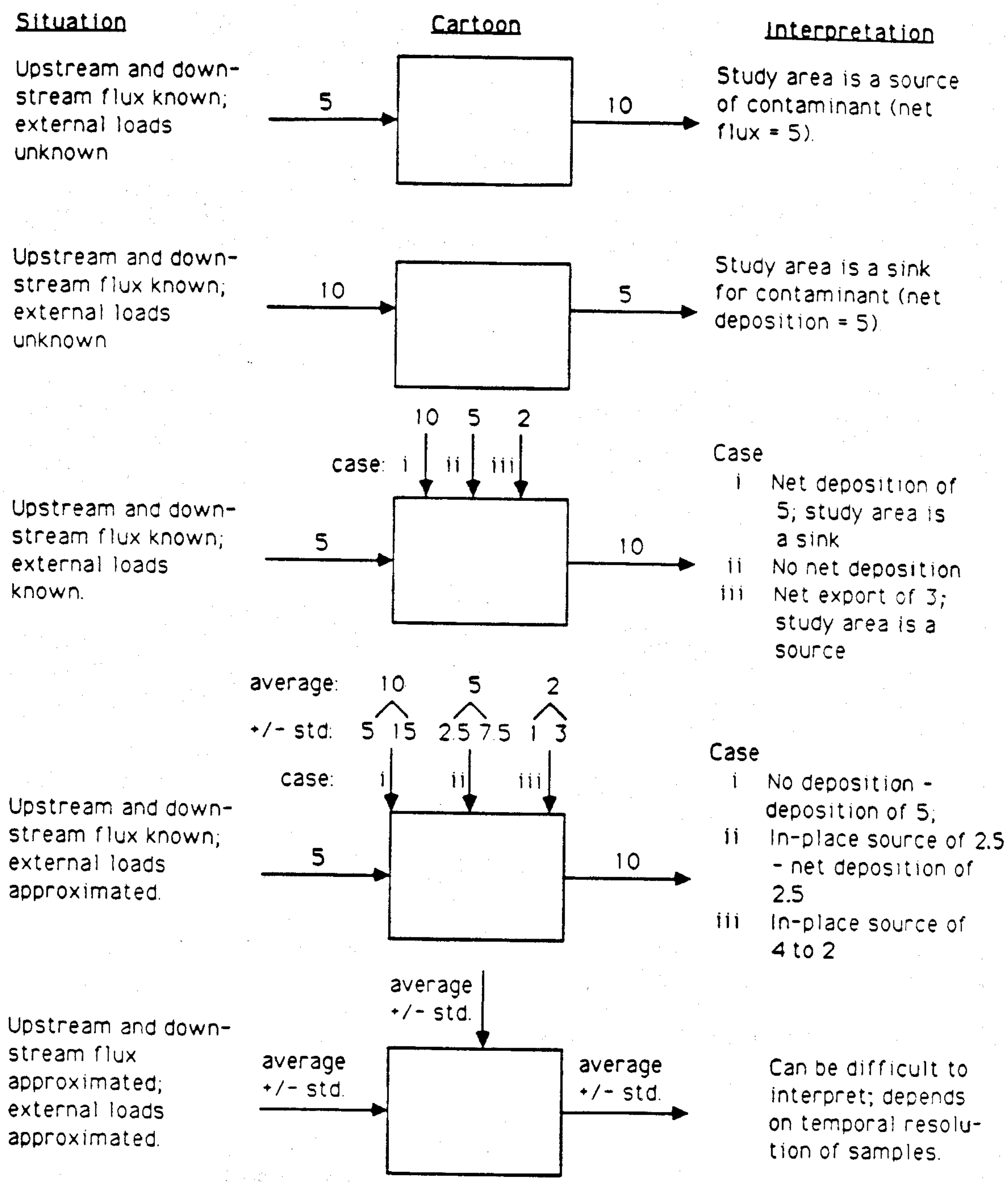

FIGURE V-1. Mass balance calculation examples.

Given a high flow condition and non-detectable concentrations, a significant portion of a contaminant mass balance can be overlooked if non-detectable concentrations are treated as zero concentration. Therefore, a method for handling non-detectables in all mass balances was devised. Details of the method used are supplied in the Modeling Workgroup Report (1).

Comparability of point source sampling between Canada (3 to 6 day sampling composites) and the U.S. (24 hour composites) was an issue. An additional issue was the use of gross loadings (U.S.-effluent only) versus net loading (effluent minus influent-Canada). The loads used in mass balance calculations that follow were those that the Point and Nonpoint Source Workgroups furnished to the Modeling Workgroup. No modifications or corrections to their numbers were made by the Modeling Workgroup.

All mass balance calculations that could be made were summarized as shown in Figure V-2. With this type of diagram the relative importance of loads can be visualized, the relative contributions of U.S. and Canadian sources can be evaluated, unknown loads can be identified, and the source-sink question can be answered for the time period in question. In mass balance diagrams the width of the arrow shafts indicate the relative importance of the average load and loss terms. Average loading terms are subdivided into Canadian and U.S. contributions. A detailed breakdown of loading figures can be obtained from the Point and Nonpoint Source Workgroup reports. At the bottom of the figure is a box that provides an interpretation of the mass balance data. Statistical conclusions are given in this box although all data leading to the interpretation are not indicated.

2. Process Models

Process-oriented models represent working hypotheses of cause and effect linkages. These simulation tools can be used to investigate the relative importance of the various processes that control the linkages. As such, process models can provide a framework for identifying needed field measurements and experimental studies. Process models have the potential for being used in more than one system because they are theoretically based. The process models developed in this study range from purely physical models of water movement to temporally and spatially complex contaminant fate and behaviour models. Verification of the latter models have been difficult due to lack of necessary and sufficient data. Nevertheless, these models are based on well documented cause and effect relationships. Thus they can be used to speculate upon the possible fate of new contaminant introductions and related organism exposures in the Connecting Channels.

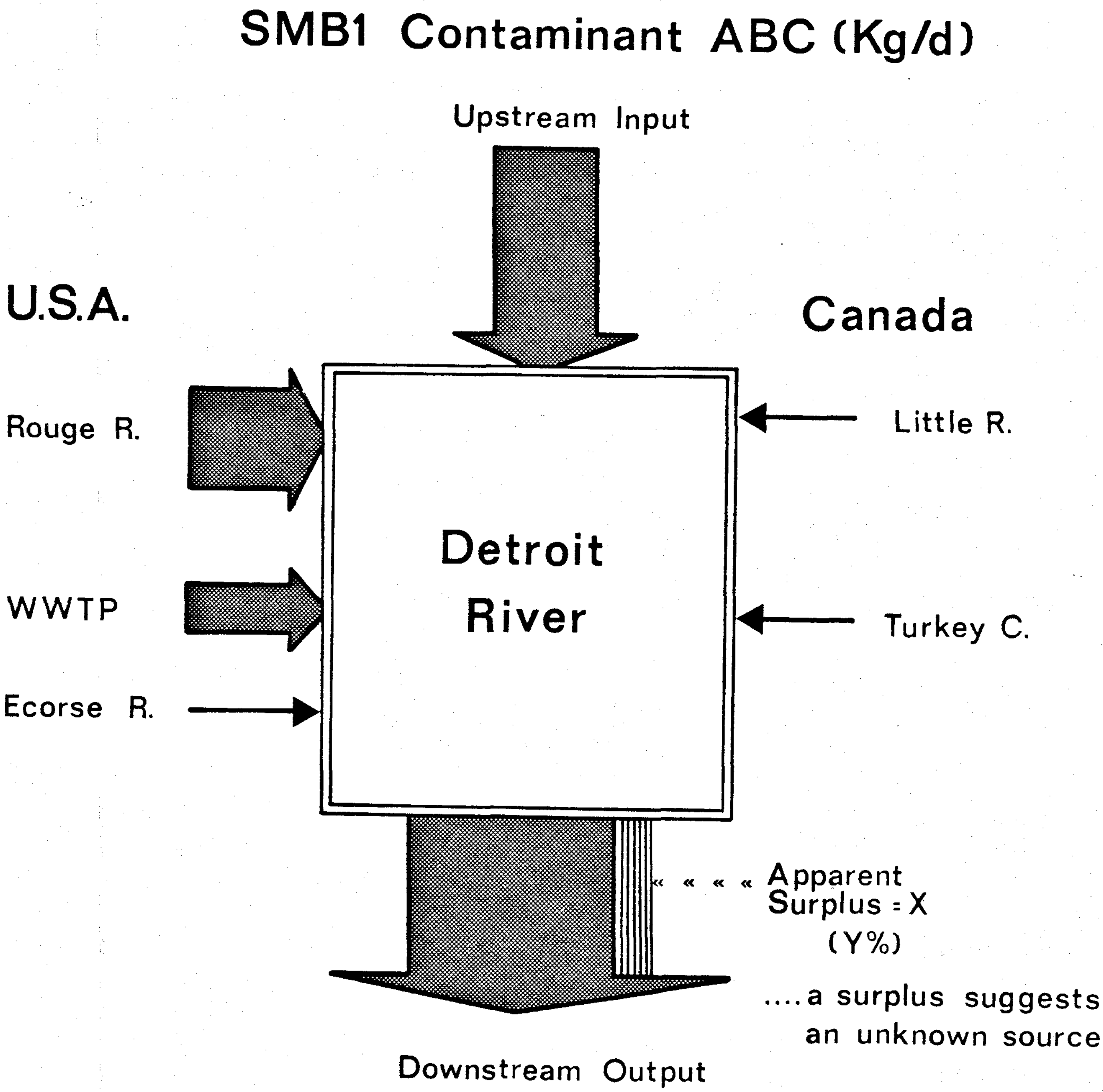

FIGURE V-2. Example of mass balance model presentations. (Detroit River Chapter VII only).

The output from process models is subject to uncertainty. Sources of uncertainty for these models include loading information, boundary conditions, initial conditions, parameter estimates (e.g., coefficient values used in process equations), and conceptual problems (e.g., are the boxes and arrows used the correct ones?). Although the Modeling Workgroup sought to conduct complete uncertainty analyses on all UGLCCS process models, time constraints and the computer resources needed for Monte Carlo-type simulations became limiting factors for most modelers. However, uncertainty analysis of models still may take place after the UGLCCS is over. Through sensitivity analyses, modelers were able to identify some parameters and processes that may require further research in order to improve contaminant fate models.

C. RECOMMENDATIONS

1. The goals of the study must be clearly defined. Recommendations for appropriate data collection and model development depend on it.

2. Goals fall into several categories: research, regulatory, remedial and political. The resource priority that each of these categories can expect to receive should be identified early on and be consistent with the goals of the study.

3. Goals must be realistic given time, personnel, financial, and laboratory capacity constraints. Realistic goals may not equate with ideal goals, but realistic goals promulgate realistic expectations.

4. Modelers are often asked to give direction to a study because models include the physical, chemical and biological processes of a system that are important for understanding its functioning and the behaviour of contaminants in it. By understanding the sensitivity of the system's behaviour to these processes, areas can be identified where data collection is most important. Modelers should be encouraged to develop "speculative" models as quickly as possible in order to perform these sensitivity analyses.

5. Monitoring and research requirements for any study should be identified in close cooperation with the modelers.

D. REFERENCE

1. Modeling Workgroup, UGLCCS 1988. Modeling Workgroup geographical area synthesis report. Draft May 1988, T.D. Fontaine (Chairman), NOAA-Great Lakes Env. Res. Lab. Ann Arbor, MI: 96 p + Append.